From biomolecular data to information

CCP5 Summer School @ University of Durham 26-27 July 2022

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Matteo Degiacomi
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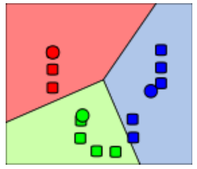
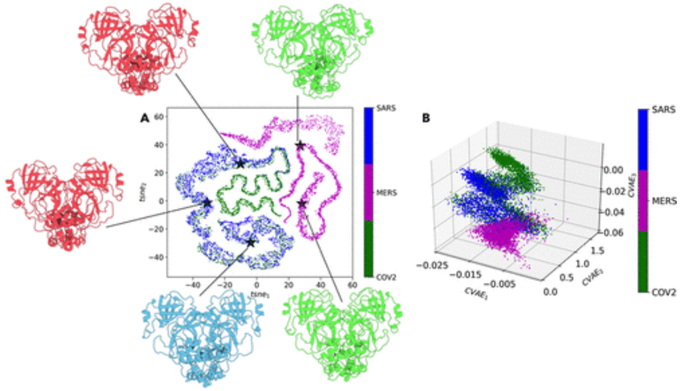
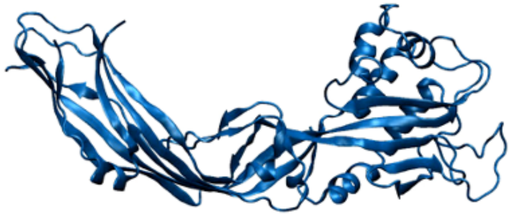






Schedule

Morning

09:00-11:00	Dimensionality Reduction theory and toy examples (TM)
11:00-11:30	☕ break ☕
11:30-12:30	ML Dimensionality Reduction application to protein simulations (MD)

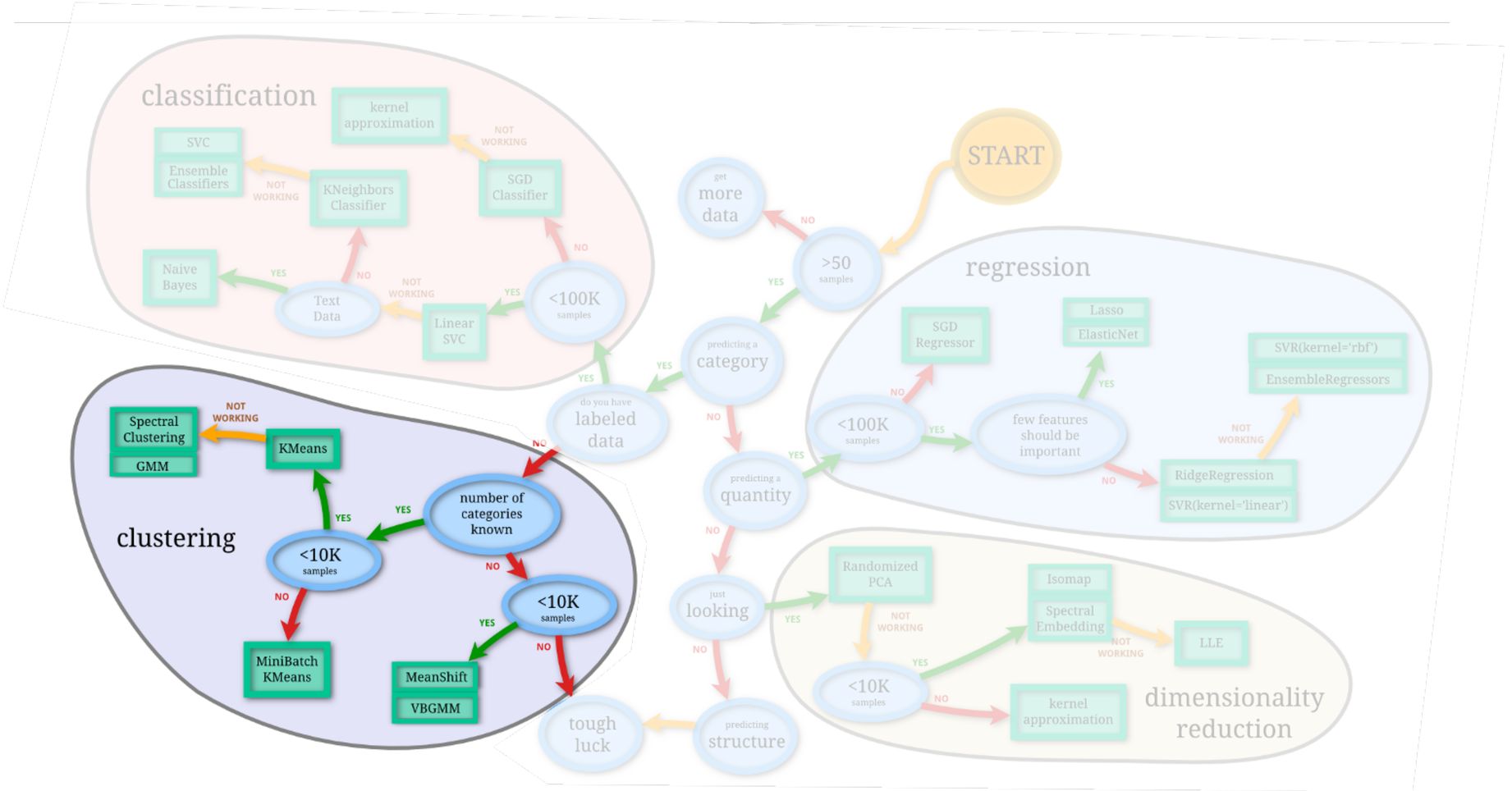
Afternoon

14:00-14:30	Clustering Theory (MD)
14:30 - 15:30	Clustering in practice (TM)
15:30 - 16:00	☕ break ☕
16:00 - 17:00	Classification problems (MD)

TM — Toni Mey

MD — Matteo Degiacomi

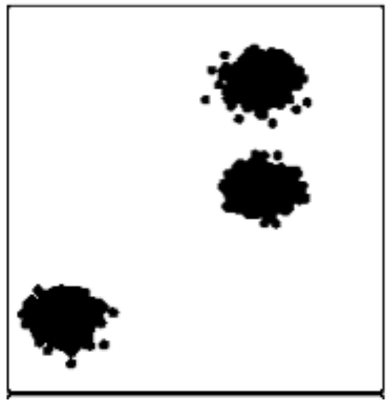
The Data Mining World — Clustering



From **scikit-learn.org**

Clustering is an unsupervised learning technique

How many clusters are there?



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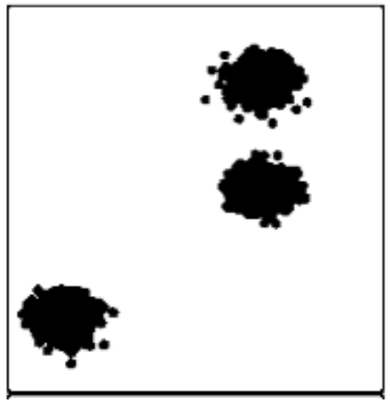

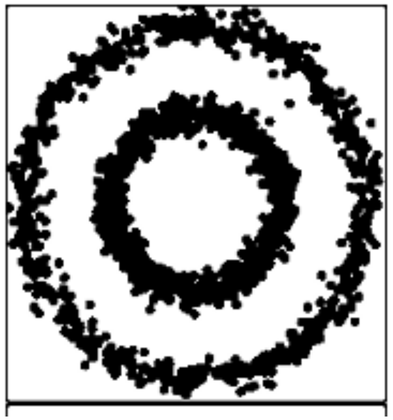

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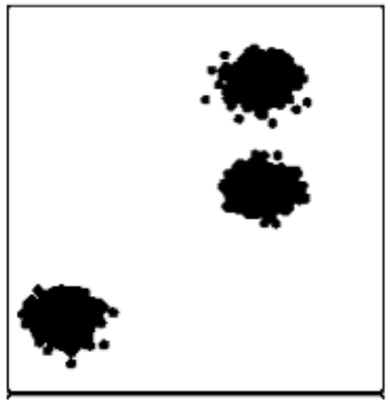

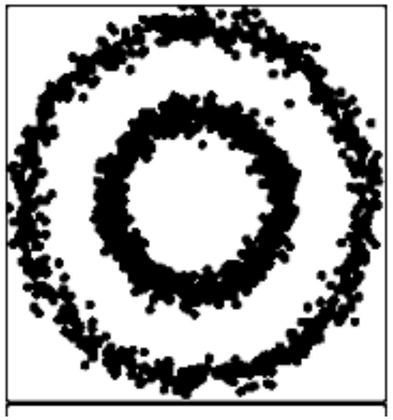

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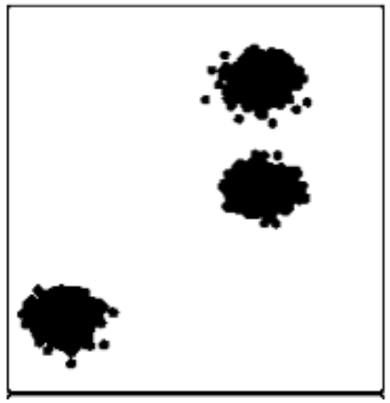

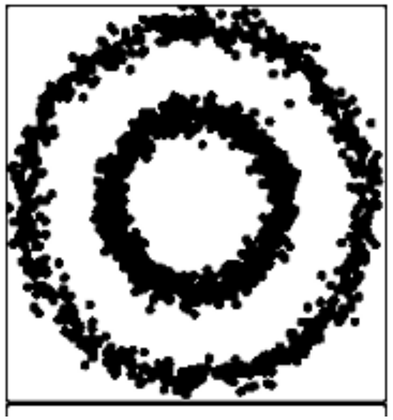

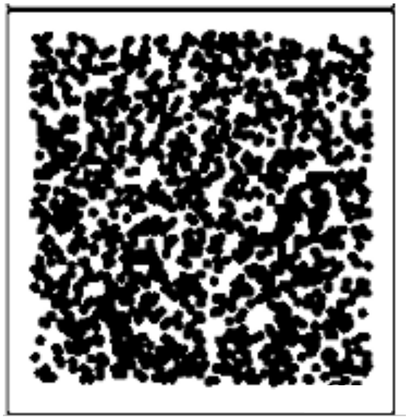

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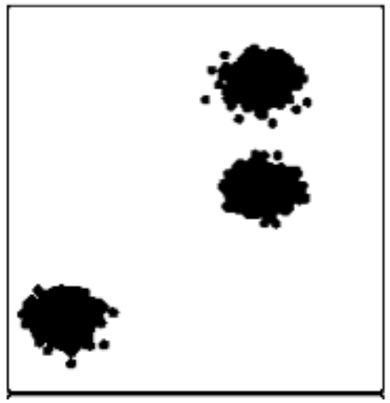
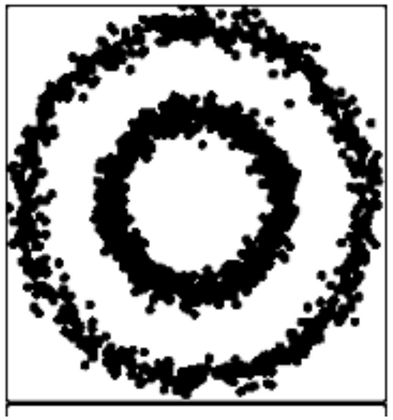
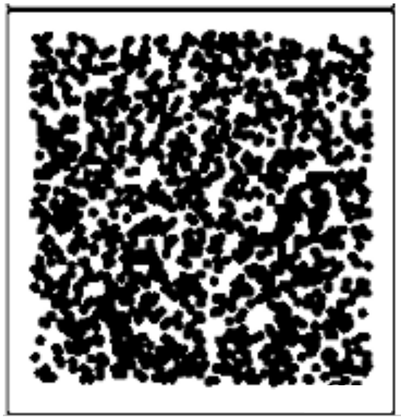
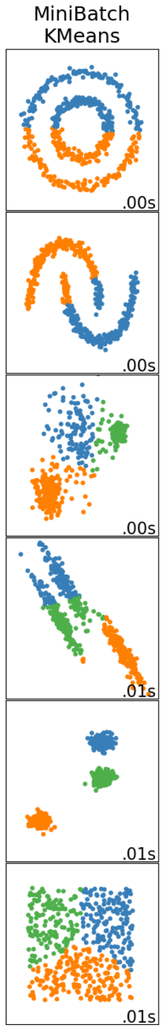






There are many different clustering algorithms



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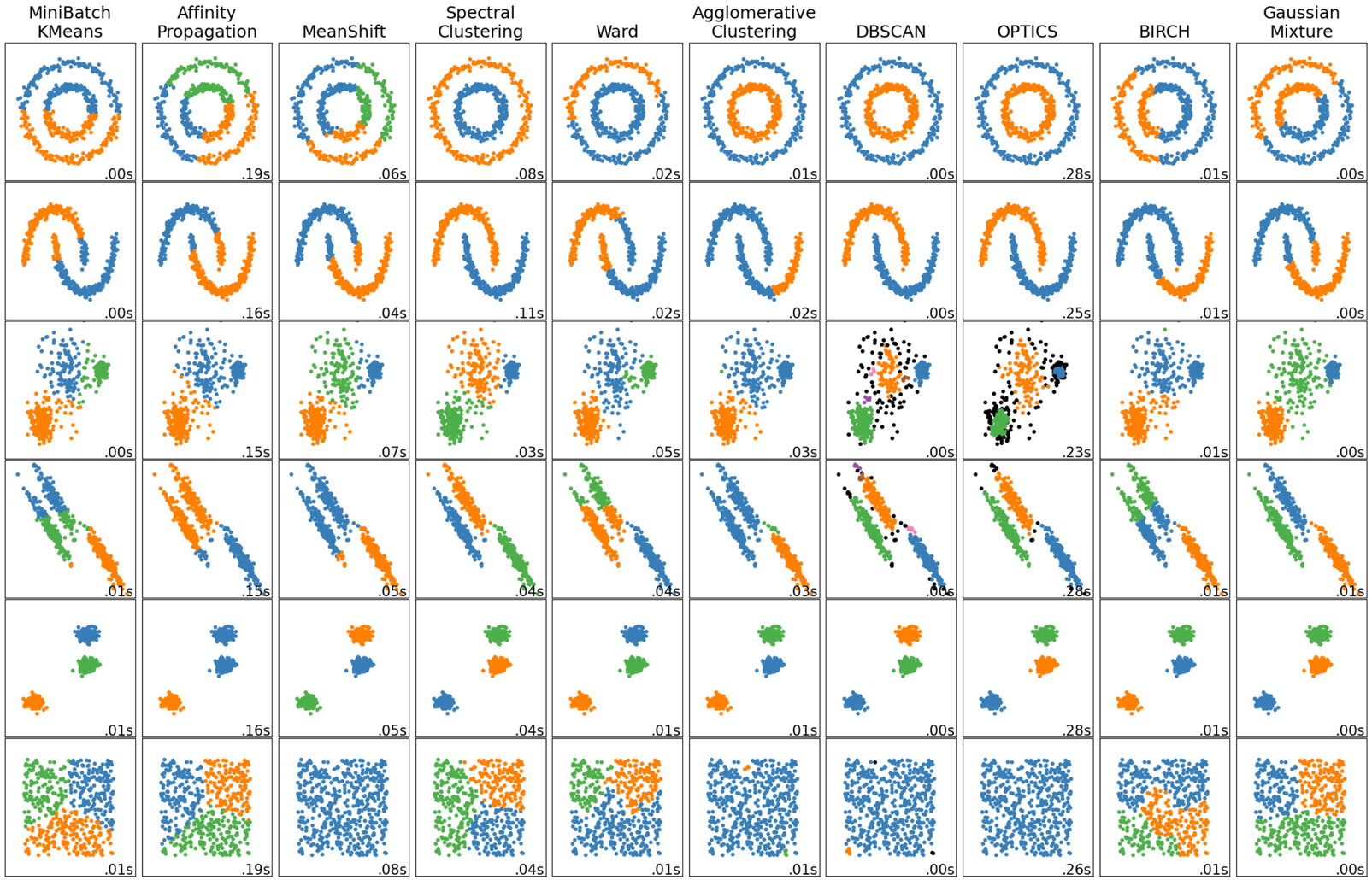
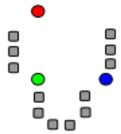
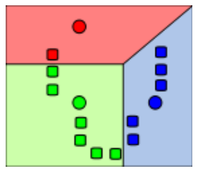


K-means, DBSCAN and spectral clustering

K-means

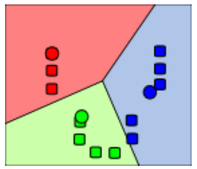


Initial guess



K-clusters are generated with the nearest mean

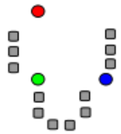
Centroid of the k-lcusters becomes the new mean



Iterate until convergence

K-means, DBSCAN and spectral clustering

K-means



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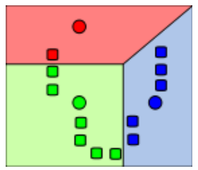

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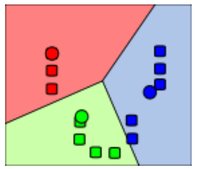

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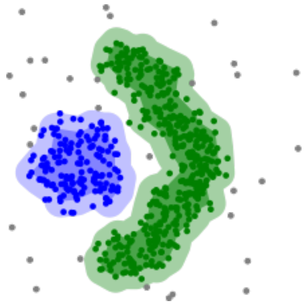
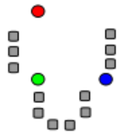
DBSCAN



1. Find the points in the ε (eps) neighbourhood of every point, and identify the core points with more than minPts neighbours.
2. Find the connected components of core points on the neighbour graph, ignoring all non-core points.
3. Assign each non-core point to a nearby cluster if the cluster is an ε (eps) neighbour, otherwise assign it to noise.

K-means, DBSCAN and spectral clustering

K-means



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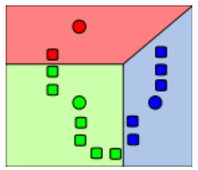

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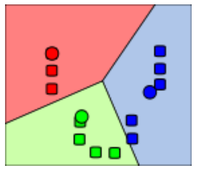

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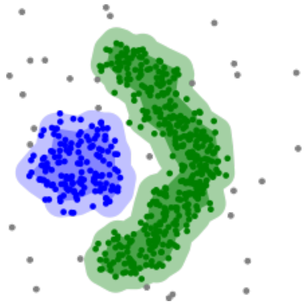

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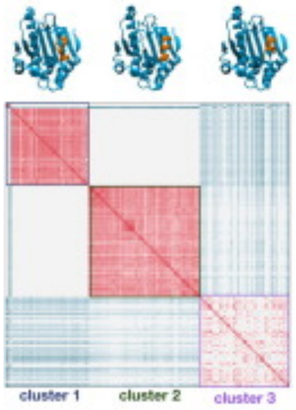
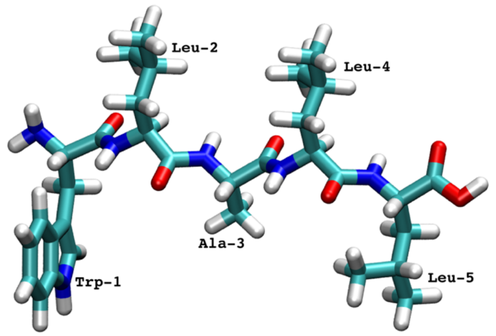
Spectral clustering

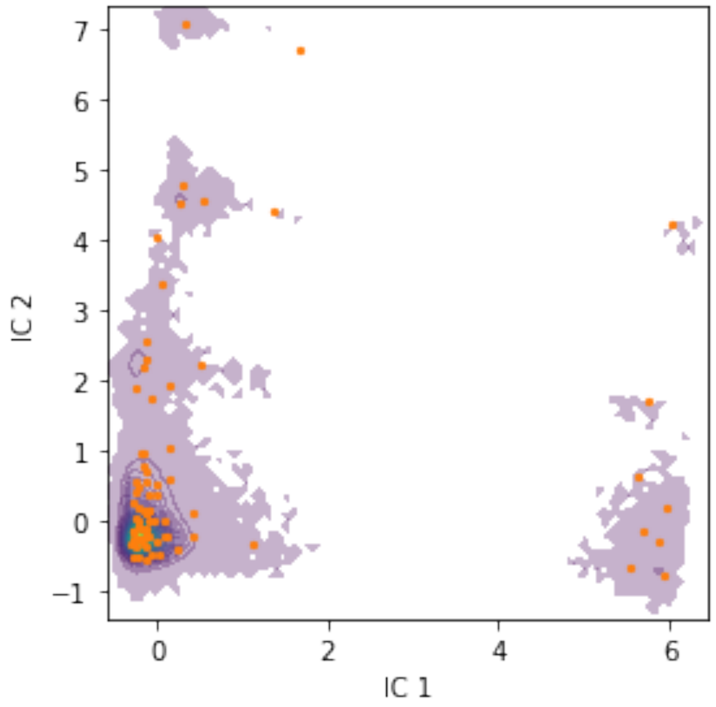


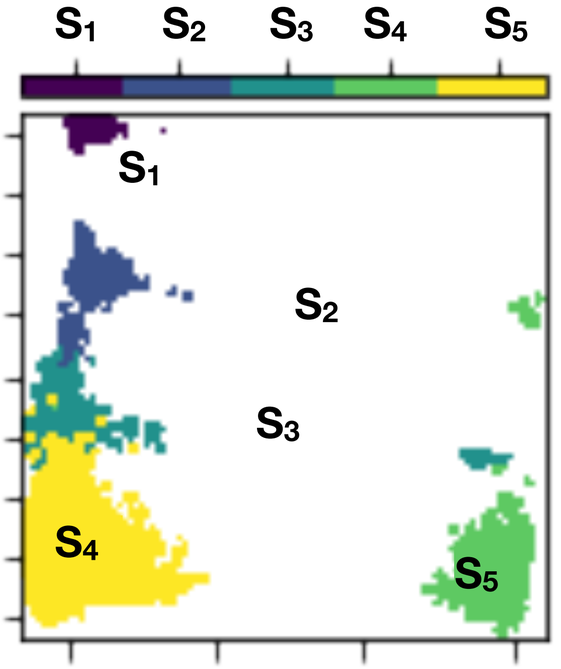
In spectral clustering clusters are found by doing an eigenvalue decomposition of the Laplacian

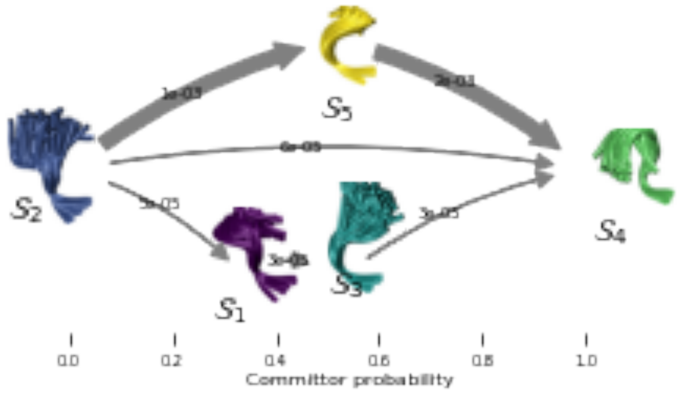
K-means example



Clustering is one of the first steps in building a Markov State Model







Post-its